

A mean-field theory of Anderson localization

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Anderson model of noninteracting disordered electrons is studied in high spatial dimensions. We find that off-diagonal one- and two-particle propagators behave as gaussian random variables w.r.t. momentum summations. With this simplification and with the electron-hole symmetry we reduce the parquet equations for two-particle irreducible vertices to a single algebraic equation for a local vertex. We find a disorder-driven bifurcation point in this equation signalling vanishing of diffusion and onset of Anderson localization. There is no bifurcation in $d = 1, 2$ where all states are localized. A natural order parameter for Anderson localization pops up in the construction.

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Understanding mobility of (free) particles in random media has been a challenging theoretical problem for many decades. It became clear from the early days of the study of systems with randomly distributed scatterers that the particle movement has a diffusive character described at long distances by a diffusion equation. A breakthrough in the conceptual perception of random systems was achieved in Ref. [1]. P. W. Anderson demonstrated there on a simple model that for a sufficiently strong disorder the particle remains confined in a finite volume and fails to diffuse to long distances. Since then, the disorder-induced absence of diffusion, called Anderson localization, has attracted a lot of attention of condensed matter theorists. In spite of years of intensive studies, the phenomenon of Anderson localization has not yet been fully understood. It is mostly due to many facets of this difficult problem.

There are two complementary tools, numerical and analytical, to tackle Anderson localization and the metal-insulator transition. Neither of them is, however, able to answer all questions about the disorder-induced vanishing of diffusion. While the former deals with finite lattices and many configurations of the random potential [2], the latter deals mostly with the thermodynamic limit and configurationally averaged quantities [3]. Although the existence of Anderson localization was proved rigorously to exist in any finite dimension if the disorder is sufficiently strong [4], both numerical and analytical approaches work preferably in rather low dimensions ($d = 2 + \epsilon$). As a consequence, a standard mean-field (high-dimensional) theory of Anderson localization is missing, except for special solutions on a Bethe lattice [5]. Even though a self-consistent, mean-field-type theory of Anderson localization was formulated [6], it was derived only within the weak-scattering, low-dimensional limit. A systematic mean-field theory should come out of the asymptotic limit to high spatial dimensions [7].

The aim of this Letter is to employ the limit to high spatial dimensions for developing a mean-field theory for the Anderson localization transition. We use the parquet

approach summing up systematically nonlocal vertex corrections to the mean-field, $d = \infty$, solution [8]. We show how the parquet equations for the irreducible two-particle vertices can be simplified and solved in the asymptotic limit to high spatial dimensions. We use the asymptotic solution of the parquet equations to build up a quantitative theory of the disorder-driven metal-insulator transition with a mean-field critical behavior, i. e., independent of the spatial dimension.

The existence or nonexistence of diffusion can be determined from the electron-hole correlation function defined from the two-particle resolvent as $\Phi(z_1, z_2; \mathbf{q}) = N^{-2} \sum_{\mathbf{k}\mathbf{k}'} G_{\mathbf{k}\mathbf{k}'}^{(2)}(z_1, z_2; \mathbf{q})$, where z_1 and z_2 are complex energies. A specific element of this function with energies $z_1 = E_F + \omega + i0^+$ and $z_2 = E_F - i0^+$, denoted $\Phi_{E_F}^{AR}(\mathbf{q}, \omega)$, is used to determine the diffusion constant [6, 9]

$$n_F D = \lim_{\omega \rightarrow 0} \frac{\omega^2}{4\pi} \nabla_{\mathbf{q}}^2 \Phi_{E_F}^{AR}(\mathbf{q}, \omega) \Big|_{\mathbf{q}=0} \quad (1)$$

where n_F is the density of states at the Fermi energy E_F . Vanishing of the diffusion constant D indicates the absence of diffusion in the system.

In systematic theories we do not approximate directly either the Green function $G^{(2)}$ or the correlation function Φ^{AR} , but rather the two-particle vertex Γ defined from [10]

$$G_{\mathbf{k}\mathbf{k}'}^{(2)}(\mathbf{q}) = G_+(\mathbf{k})G_-(\mathbf{k} + \mathbf{q})[\delta(\mathbf{k} - \mathbf{k}') + \Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q})G_+(\mathbf{k}')G_-(\mathbf{k}' + \mathbf{q})]$$

where $G_{\pm}(\mathbf{k}) \equiv G(\mathbf{k}, z_{\pm})$ are averaged one-particle resolvents.

The simplest theory for strongly disordered systems is the coherent-potential approximation (CPA), being an exact solution in $d = \infty$. Only the diagonal part of the one-electron resolvent $G(z) = N^{-1} \sum_{\mathbf{k}} G(\mathbf{k}, z)$ is relevant in the CPA, since it completely neglects coherence between spatially distinct scatterings. It is a consistent mean-field theory only for one-electron functions. Nonlocal parts of two-particle functions in high dimensions do

not vanish. The off-diagonal elements of the one-electron propagators cannot be neglected and have to be taken explicitly into consideration [7]. Further on, the CPA, due to its local character, is degenerate and cannot distinguish between scatterings of electrons and holes. To be able to resolve various types of two-particle scatterings in noninteracting systems we have to go beyond the mean-field, local approximation.

A systematic (diagrammatic) expansion around the $d = \infty$ limit can be performed by using the off-diagonal one-electron CPA resolvent $\bar{G}(\mathbf{k}, z) \equiv G(\mathbf{k}, z) - G(z)$. Three nonequivalent Bethe-Salpeter equations with non-local propagators can be constructed for the full vertex Γ [8]. Here we will use only the Bethe-Salpeter equations from the electron-hole and the electron-electron scattering channels [11]. They can be represented as

$$\begin{aligned}\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) &= \bar{\Lambda}_{\mathbf{k}\mathbf{k}'}^{eh}(\mathbf{q}) + \frac{1}{N} \sum_{\mathbf{k}''} \bar{\Lambda}_{\mathbf{k}\mathbf{k}''}^{eh}(\mathbf{q}) \\ &\quad \times \bar{G}_+(\mathbf{k}'') \bar{G}_-(\mathbf{k}'' + \mathbf{q}) \Gamma_{\mathbf{k}''\mathbf{k}'}(\mathbf{q}), \\ \Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) &= \bar{\Lambda}_{\mathbf{k}\mathbf{k}'}^{ee}(\mathbf{q}) + \frac{1}{N} \sum_{\mathbf{k}''} \bar{\Lambda}_{\mathbf{k}\mathbf{k}''}^{ee}(\mathbf{q} + \mathbf{k}' - \mathbf{k}'') \\ &\quad \times \bar{G}_+(\mathbf{k}'') \bar{G}_-(\mathbf{Q} - \mathbf{k}'') \Gamma_{\mathbf{k}''\mathbf{k}'}(\mathbf{q} + \mathbf{k} - \mathbf{k}''),\end{aligned}\quad (2a)$$

respectively. We used bar in the irreducible vertices $\bar{\Lambda}^{eh}$ and $\bar{\Lambda}^{ee}$ to indicate that the Bethe-Salpeter equations are constructed with the off-diagonal resolvents only. Hence, in the infinite-dimensional case $\bar{G}_{\pm}(\mathbf{k}) = 0$ and $\bar{\Lambda}^{eh, ee} = \gamma$, where γ is the full local CPA vertex [8]. For simplicity of notation we denoted $\mathbf{Q} \equiv \mathbf{q} + \mathbf{k} + \mathbf{k}'$. Notice that \mathbf{q} is the momentum conserved for scatterings in the electron-hole channel, Eq. (2a), while \mathbf{Q} is conserved in the electron-electron channel, Eq. (2b).

To reach the strong-disorder limit with a diffusionless regime we have to determine the irreducible vertices $\bar{\Lambda}^{eh}$ and $\bar{\Lambda}^{ee}$ self-consistently. The parquet construction provides a suitable framework for this purpose. It is based on the observation that *reducible diagrams* in one channel are *irreducible* in the other, topologically distinct channels. If we approximate the vertex irreducible in all channels by the local CPA vertex γ , take into account only the *eh* and *ee* channels, and realize that the full vertex is a sum of reducible and irreducible vertices in any channel, we end up with a fundamental parquet equation

$$\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \bar{\Lambda}_{\mathbf{k}\mathbf{k}'}^{eh}(\mathbf{q}) + \bar{\Lambda}_{\mathbf{k}\mathbf{k}'}^{ee}(\mathbf{q}) - \gamma. \quad (3)$$

The minus sign at the CPA vertex compensates for the identical local part in both $\bar{\Lambda}^{eh}$ and $\bar{\Lambda}^{ee}$. A couple of (nonlinear) parquet equations determining the irreducible vertices $\bar{\Lambda}^{eh}$ and $\bar{\Lambda}^{ee}$ as functions of γ and \bar{G}_{\pm} are obtained by replacing the full vertex Γ in Eqs. (2) by Eq. (3).

Prior to solving the parquet equations for $\bar{\Lambda}^{eh}$ and $\bar{\Lambda}^{ee}$ we utilize the electron-hole symmetry expressed as

an identity for two-particle vertices $\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \Gamma_{\mathbf{k}\mathbf{k}'}(-\mathbf{q} - \mathbf{k} - \mathbf{k}')$ and $\bar{\Lambda}_{\mathbf{k}\mathbf{k}'}^{ee}(\mathbf{q}) = \bar{\Lambda}_{\mathbf{k}\mathbf{k}'}^{eh}(-\mathbf{q} - \mathbf{k} - \mathbf{k}')$. The electron-hole transformation maps Eq. (2a) onto Eq. (2b). The two-particle electron-hole symmetry is a consequence of the time-reversal invariance the one-electron resolvent $\bar{G}(\mathbf{k}, z) = \bar{G}(-\mathbf{k}, z)$ used in the Bethe-Salpeter equations (2). This symmetry actually reduces the number of parquet equations to a single nonlinear integral equation for $\bar{\Lambda}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) \equiv \bar{\Lambda}_{\mathbf{k}\mathbf{k}'}^{ee}(\mathbf{q}) = \bar{\Lambda}_{\mathbf{k}\mathbf{k}'}^{eh}(-\mathbf{q} - \mathbf{k} - \mathbf{k}')$.

Generally, the parquet equations are unsolvable due to momentum convolutions in the Bethe-Salpeter equations. The limit to high spatial dimensions leads to suppression of spatial fluctuations resulting in simplifications of momentum convolutions [12]. We take advantage of these simplifications. We start with the leading asymptotic term in the off-diagonal propagator $\bar{G}(\mathbf{k}, z)$ that on a d -dimensional hypercubic lattice with the hopping amplitude t reads

$$\begin{aligned}\bar{G}(\mathbf{k}, z) &\doteq \frac{t}{\sqrt{d}} \sum_{\nu=1}^d \cos(k_{\nu}) \int d\epsilon \rho(\epsilon) G(z - \Sigma(z) - \epsilon)^2 \\ &= tx(\mathbf{k}) \langle G(z)^2 \rangle, \quad (4)\end{aligned}$$

where ρ is the density of states and Σ the local (CPA) self-energy. We replace the off-diagonal one-electron propagators in the parquet equations with this asymptotic representation.

The simplest and most important convolution is a two-particle bubble $\bar{\chi}(\mathbf{q}) = N^{-1} \sum_{\mathbf{k}} \bar{G}_+(\mathbf{k}) \bar{G}_-(\mathbf{k} + \mathbf{q})$. Its asymptotic behavior can be found from the following formula

$$\frac{1}{N} \sum_{\mathbf{k}} x(\mathbf{k}) x(\mathbf{k} + \mathbf{q}) = \frac{1}{2} X(\mathbf{q}) = \frac{1}{2d} \sum_{\nu=1}^d \cos(q_{\nu}) \quad (5a)$$

where we denoted $X(\mathbf{q})$ a two-particle (bosonic) dispersion function. Other possible convolutions of the generic fermionic and bosonic dispersion functions are

$$\frac{1}{N} \sum_{\mathbf{q}'} X(\mathbf{q}' + \mathbf{q}) x(\mathbf{q}' + \mathbf{k}) = \frac{1}{2d} x(\mathbf{q} - \mathbf{k}), \quad (5b)$$

$$\frac{1}{N} \sum_{\mathbf{q}'} X(\mathbf{q}' + \mathbf{q}_1) X(\mathbf{q}' + \mathbf{q}_2) = \frac{1}{2d} X(\mathbf{q}_1 - \mathbf{q}_2). \quad (5c)$$

We can see that the fermionic and bosonic dispersion functions form a closed algebra with respect to momentum summations. The elementary convolutions (5) manifest the generation of the factor d^{-1} due to mixing of two-particle propagations from different scattering channels. The dispersion functions then behave in the leading asymptotic order of d^{-1} as *gaussian random variables* when momentum summations are performed.

To make the calculations in high spatial dimensions more mean-field-like, we replace the bare fermionic and bosonic dispersion functions with the respective off-diagonal one- and two-particle propagators. That is, we

use \bar{G} instead of x and $\bar{\chi}$ instead of X . These quantities are directly proportional in the leading asymptotic order. Without loosing the asymptotic accuracy we can extend relations (5) to genuine mean-field expressions $N^{-1} \sum_{\mathbf{q}'} \bar{\chi}(\mathbf{q}' + \mathbf{q}) \bar{G}_{\pm}(\mathbf{q}' + \mathbf{k}) = W \bar{G}_{\pm}(\mathbf{q} - \mathbf{k})/4d$, $N^{-1} \sum_{\mathbf{q}} \bar{\chi}(\mathbf{q} + \mathbf{q}_1) \bar{\chi}(\mathbf{q} + \mathbf{q}_2) = W \bar{\chi}(\mathbf{q}_1 - \mathbf{q}_2)/4d$, where we used $W = t^2 \langle G_+^2 \rangle \langle G_-^2 \rangle$.

It is evident from Eq. (4) and Eq. (5) that the two-particle vertices can be represented as functions of the generic off-diagonal fermionic $\bar{G}(\mathbf{k})$ and bosonic $\bar{\chi}(\mathbf{q})$ functions. To find the leading high-dimensional asymptotics of the solution of the parquet equation for $\bar{\Lambda}_{\mathbf{k}\mathbf{k}'}(\mathbf{q})$ we keep only the leading d^{-1} terms for each specific momentum dependence of the vertex. It is easy to demonstrate that the parquet equation then simplifies in the leading asymptotic limit $d \rightarrow \infty$ to an algebraic equation

$$\bar{\Lambda}_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \bar{\Lambda}(\mathbf{q}) = \gamma + \bar{\Lambda}_0 \frac{\bar{\Lambda}_0 \bar{\chi}(\mathbf{q})}{1 - \bar{\Lambda}_0 \bar{\chi}(\mathbf{q})} \quad (6a)$$

where $\bar{\Lambda}_0 = N^{-1} \sum_{\mathbf{q}} \bar{\Lambda}(\mathbf{q})$. The high-dimensional irreducible two-particle vertex is completely determined from a single local parameter $\bar{\Lambda}_0$ and the two-particle bubble $\bar{\chi}(\mathbf{q})$. Summing both sides of Eq. (6a) over momenta we obtain

$$\bar{\Lambda}_0 = \gamma + \bar{\Lambda}_0 \frac{1}{N} \sum_{\mathbf{q}} \frac{\bar{\Lambda}_0 \bar{\chi}(\mathbf{q})}{1 - \bar{\Lambda}_0 \bar{\chi}(\mathbf{q})}. \quad (6b)$$

Equations (6) were derived from the leading high-dimensional asymptotics, but can be used in any finite dimension. It is, however, mandatory that the proper d -dimensional momentum summation is used on a d -dimensional lattice. We cannot directly use the gaussian rules to evaluate the summation over momenta in d dimensions as we did during the derivation of these equations. The integrand would be singular (nonintegrable) in the gaussian evaluation. To assess the asymptotic high-dimensional behavior of the two-particle irreducible vertex we have to realize that in deriving Eq. (6) each independent one-dimensional momentum integration over the components q_i with $i = 1, 2, \dots, d$ can contain maximally squares of the dispersion to remain within the leading asymptotics. Hence, on a d -dimensional lattice we can build maximally d pairs of the two-particle bubbles $\bar{\chi}$. The integrand in Eq. (6b) therefore collapses to a polynomial of order d . Using the gaussian integration rules we explicitly obtain

$$f_d(a) = \frac{1}{N} \sum_{\mathbf{q}} \frac{\bar{\Lambda}_0 \bar{\chi}(\mathbf{q})}{1 - \bar{\Lambda}_0 \bar{\chi}(\mathbf{q})} \Big|_d \equiv \sum_{n=1}^d \frac{(2n)!}{(2d)^n n!} (a)^n$$

where we denoted $a = W^2 \bar{\Lambda}_0^2/8$. The asymptotic limit of the sum $f_{d \rightarrow \infty}(a)$ converges for $a < 1/2$, i. e., for $\bar{\Lambda}_0^2 < 4/W^2$. The critical value of the randomness

$\gamma^2 = 4/W^2$ defines an ultimate upper bound beyond which perturbation theory around $d = \infty$ in powers of d^{-1} does not converge and becomes nonanalytic. In realistic models, however, such an extreme value cannot be reached, apart from tiny regions around band edges and in satellite bands.

The one-electron functions G, Σ and the local two-particle vertex γ entering Eqs. (6) were assumed to be taken from the CPA. There we have $\gamma = \lambda/(1 - \lambda G_+ G_-)$ and $\lambda = (\Sigma_+ - \Sigma_-)/(G_+ - G_-)$. If we analogously define $\bar{\Lambda}_0 = \Lambda_0/(1 - \Lambda_0 G_+ G_-)$ and $\chi(\mathbf{q}) = \bar{\chi}(\mathbf{q}) + G_+ G_-$ we can represent the asymptotic form of the full two-particle vertex as follows

$$\Gamma_{\mathbf{k}\mathbf{k}'}(\mathbf{q}) = \gamma + \Lambda_0 \left[\frac{\bar{\Lambda}_0 \bar{\chi}(\mathbf{q})}{1 - \Lambda_0 \chi(\mathbf{q})} + \frac{\bar{\Lambda}_0 \bar{\chi}(\mathbf{k} + \mathbf{k}' + \mathbf{q})}{1 - \Lambda_0 \chi(\mathbf{k} + \mathbf{k}' + \mathbf{q})} \right]. \quad (7)$$

The full nonlocal CPA vertex can be recovered from the above expression if we put $\bar{\Lambda}_0 = \gamma$ and neglect the last term on the r.h.s. of Eq. (7). The term neglected in the CPA, however, restores the electron-hole symmetry in the asymptotic vertex in high dimensions.

Up to now we have analyzed the two-particle asymptotics with the one-electron propagators fixed by the CPA. To reproduce diffusion in this approach we have to match correctly the irreducible vertex calculated from the parquet equations (6) and the one-electron self-energy. We hence have to go beyond the CPA even in the one-electron propagators. To do so consistently we use the Ward identity and determine the imaginary part of the self-energy from the two-particle irreducible vertex via

$$\Im \Sigma(E + i0^+) = \Lambda_0(E + i0^+, E - i0^+) \Im G(E + i0^+). \quad (8)$$

The real part of the self-energy is determined from the Kramers-Kronig relation [8]. Equation (8) completes the parquet equation (6b). Both equations together with the Kramers-Kronig relation have to be solved simultaneously to achieve full self-consistence between Λ_0 and G calculated from Σ via the Dyson equation.

The redefinition of the self-energy in Eq. (8) is important, since only with it we recover the diffusion pole in the vertex functions. That is, we obtain $\Lambda_0(E + i0^+, E - i0^+) \chi(\mathbf{0}) = 1$, whenever the parquet equation (6b) allows for a positive solution. The existence of the diffusion pole is essential for the diffusion constant from Eq. (1) to be non-zero (positive). We can immediately conclude from simple power counting in the momentum integral of Eq. (6b) that there is no positive solution for $\bar{\Lambda}_0(E + i0^+, E - i0^+)$ in low dimensions, $d = 1, 2$, since the diffusion pole would be nonintegrable. Consequently, no diffusion pole can exist and the diffusion constant from Eq. (1) vanishes in $d = 1, 2$.

In higher dimensions we can expand the r.h.s. of Eq. (6b) in powers of the local vertex $\bar{\Lambda}_0$. We then obtain

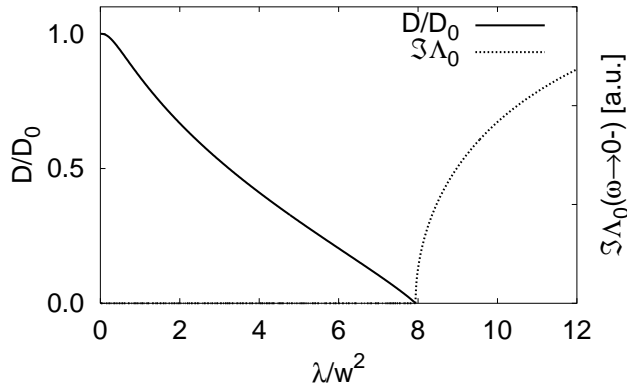


FIG. 1: Diffusion constant D and the order parameter in the localized phase $\Im\Lambda_0$ calculated from Eq. (9). We used a semielliptic energy band with the bandwidth $2w$, the self-consistent Born approximation for the self-energy, and set $C_d = 0.1W^2$.

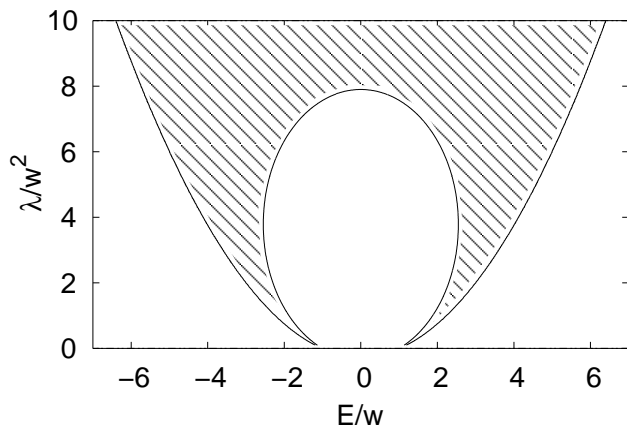


FIG. 2: Phase diagram for the same setting as in Fig. 1. The hatched area denotes localized states.

a mean-field-like cubic equation

$$\bar{\Lambda}_0 = \gamma + C_d \bar{\Lambda}_0^3 \quad (9)$$

with $C_d = \lim_{\bar{\Lambda}_0 \rightarrow 0} N^{-1} \sum_{\mathbf{q}} \bar{\chi}(\mathbf{q})^2 / (1 - \bar{\Lambda}_0 \bar{\chi}(\mathbf{q}))^2$. This constant is generally a decreasing function of the spatial dimension d and approaches zero in the limit $d \rightarrow \infty$ via $C_d \sim W^2/8d$. Due to the existence of the diffusion pole in Eq. (6b) the constant C_d becomes infinite in $d \leq 4$. Equation (9) derived from a Taylor expansion in the local vertex $\bar{\Lambda}_0$ does not survive in this form to low dimensions.

Equation (9) has generally three solutions for $\bar{\Lambda}_0(E + i0^+, E - i0^+)$. For sufficiently small disorder strengths, $\gamma < \gamma_c$, all three solutions are real. A perturbative solution is of order γ , while two nonperturbative solutions are of order $\pm\sqrt{1/C_d}$. The perturbative solution increases and the module of the nonperturbative ones decreases with increasing the disorder strength. At a critical randomness $3C_d\bar{\Lambda}_0^2 = 1$, or equivalently $\gamma_c = \sqrt{4/27C_d}$, the

two positive solutions merge and move into the complex plane for $\gamma > \gamma_c$. Disappearance of positive solutions for $\bar{\Lambda}_0(E + i0^+, E - i0^+)$ leads to suppression of the diffusion pole and simultaneously to vanishing of the diffusion constant. Quantity $\Im\bar{\Lambda}_0(E + i0^+, E - i0^+)$, emerging beyond the critical point in the localized phase ($\gamma > \gamma_c$), plays the role of an order parameter for Anderson localization, see Fig. 1. A typical phase diagram for localized-extended states calculated from Eq. (9) is plotted in Fig. 2. Although the mean-field equation (9) does not predict the precise position of the mobility edges, it determines the mean-field universal properties accurately.

To conclude, we derived a mean-field approximation for two-particle irreducible vertices motivated and justified by the asymptotic limit to high dimensions. We succeeded in deriving an algebraic equation for the local irreducible vertex with a bifurcation point at which the diffusion constant vanishes and a real irreducible vertex becomes complex. A fully consistent and controllable mean-field-like theory of the disorder-driven vanishing of diffusion and Anderson localization was thereby achieved. It correctly reproduces the low and high-dimensional limits and allows for further systematic improvements.

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